Estrone, hexanoate

Inchi: InChI=1S/C24H32O3/c1-3-4-5-6-23(26)27-17-8-10-18-16(15-17)7-9-20-19(18)13-14-24(2
InchiKey: KAUHLUBURUDAPE-UHFFFAOYSA-N
Formula: C24H32O3
SMILES: CCCCCC(=O)Oc1ccc2c(c1)CCC1C2CCC2(C)C(=O)CCC12
Mol. weight [g/mol]: 368.51

Physical Properties

Property code	Value	Unit	Source
gf	32.69	kJ/mol	Joback Method
hf	-506.62	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	84.64	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.597		Crippen Method
mcvol	301.690	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
tb	953.60	K	Joback Method
tc	1191.07	K	Joback Method
tf	618.52	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.65	J/mol×K	953.60	Joback Method
cpg	1092.43	J/mol×K	993.18	Joback Method
cpg	1114.84	J/mol×K	1032.76	Joback Method
cpg	1137.09	J/mol×K	1072.33	Joback Method
cpg	1159.40	J/mol×K	1111.91	Joback Method
cpg	1181.99	J/mol×K	1151.49	Joback Method
cpg	1205.07	J/mol×K	1191.07	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume